

4-Isobutylmorpholine
10315-98-7 | DTXSID30145675

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.74e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.51e-01

Confidence level: 5.51e-01

Nearest Neighbors from the Training Set

Image not found

4-Isobutylmorpholine

Measured: 1.95e-01

Predicted: 3.74e-01

Image not found

N-Ethylmorpholine

Measured: 8.68

Predicted: 6.40

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1,2-Bis(2-chloroethoxy)ethane

Measured: 1.01e-01

Predicted: 1.12e-01

Image not found

Methanediamine, N,N,N',N'-
tetraethyl-

Measured: 6.32e-01

Predicted: 1.89e-01